

2-Phenylethyl acetate
103-45-7 | DTXSID7044506

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -22.7 °C

Global applicability domain: Inside

Local applicability domain index: 9.78e-01

Confidence level: 6.58e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Phenylethyl acetate</div> <div>Measured: -31.1</div> <div>Predicted: -22.7</div>	<div>Image not found</div> <div>Ethyl phenylacetate</div> <div>Measured: -29.4</div> <div>Predicted: -23.1</div>	<div>Image not found</div> <div>Propyl benzoate</div> <div>Measured: -51.6</div> <div>Predicted: -23.7</div>
<div>Image not found</div> <div>3,4-Xylyl acetate</div> <div>Measured: 22.0</div> <div>Predicted: -12.6</div>	<div>Image not found</div> <div>Methyl 2,4-dimethylbenzoate</div> <div>Measured: -2.00</div> <div>Predicted: -13.4</div>	